Adiabatic Product Expansion

Ali Mostafazadeh*

Theoretical Physics Institute, University of Alberta,
Edmonton, Alberta, Canada T6G 2J1.

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Abstract

The time-evolution operator for an explicitly time-dependent Hamiltonian is expressed as the product of a sequence of unitary operators. These are obtained by successive time-dependent unitary transformations of the Hilbert space followed by the adiabatic approximation at each step. The resulting adiabatic product expansion yields a generalization of the quantum adiabatic approximation. Furthermore, it leads to an infinite class of exactly solvable models.

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Consider the dynamics of a quantum mechanical system whose Hamiltonian $H = H(\tau)$ is explicitly time-dependent. The evolution of a state vector $|\psi(\tau)\rangle$ is governed by the Schrödinger equation:

$$i\hbar|\dot{\psi}(\tau)\rangle = H(\tau)\,|\psi(\tau)\rangle\ , \qquad |\psi(0)\rangle = |\psi_0\rangle\ , \tag{1}$$

where a dot means a time-derivative. Alternatively, one has $|\psi(\tau)\rangle = U(\tau)|\psi_0\rangle$, where

$$U(\tau) = \mathcal{T}\ e^{-\frac{i}{\hbar}\int_0^\tau H(t)\,dt} \tag{2}$$

is the time-evolution operator. Here $\mathcal{T}$ denotes the time-ordering operator. The purpose of this article is to express $U(\tau)$ as the product of a sequence of unitary operators each of

*E-mail: alimos@phys.ualberta.ca

which is the adiabatically approximate time-evolution operator in some adiabatically moving frame.

In order to construct these unitary operators, let us separate the adiabatic part $U^{(0)}(\tau)$ of the exact time-evolution operator:

$$U(\tau) = U^{(0)}(\tau)\, V^{(1)}(\tau)\ . \tag{3}$$

$U^{(0)}(\tau)$ is defined by

$$U^{(0)}(\tau) \ := \ \sum_n e^{i\alpha_n(\tau)}\, |n;\tau\rangle\langle n;0|\ , \tag{4}$$

$$\alpha_n(\tau) \ := \ \delta_n(\tau) + \gamma_n(\tau)\,, \tag{5}$$

$$\delta_n(\tau) \ := \ -\frac{1}{\hbar}\int_0^\tau E_n(t)dt\,, \qquad \gamma_n(\tau) \ := \ i\int_0^\tau \langle n;t|\frac{d}{dt}|n;t\rangle\, dt\ , \tag{6}$$

where $|n;t\rangle$ are instantaneous eigenvectors of the Hamiltonian $H(t)$ with eigenvalue $E_n(t)$, i.e.,

$$H(t)|n;t\rangle = E_n(t)\,|n;t\rangle\ . \tag{7}$$

Throughout this article, it is assumed that the energy spectrum is discrete, all the eigenvalues of the Hamiltonian are non-degenerate and there is no level-crossing.

The adiabatic time-evolution operator $U^{(0)}(\tau)$ as defined by (4) includes the effects of Berry's geometric phase [1], through the phase angles $\gamma_n(t)$. The operator $V^{(1)}(\tau)$ includes the non-adiabatic effects. As $U^{(0)}(\tau)$ is unitary, Eq. (3) may be viewed as the definition of $V^{(1)}(\tau)$.

Next consider an arbitrary time-dependent unitary transformation of the state vectors: $|\psi(\tau)\rangle \to |\psi'(\tau)\rangle := \mathcal{U}(\tau)|\psi(\tau)\rangle$. This may be viewed as transforming to a "moving frame" of reference. In the "moving frame" the state vectors also satisfy a Schrödinger equation with a new Hamiltonian $\mathcal{H}(\tau)$. This is related to $H(\tau)$ according to

$$\mathcal{H}(\tau) = \mathcal{U}(\tau)\, H(\tau)\, \mathcal{U}^\dagger(\tau) - i\hbar\, \mathcal{U}(\tau)\, \dot{\mathcal{U}}^\dagger(\tau)\ . \tag{8}$$

Now let us set $\mathcal{U}(\tau) = U^{(0)\dagger}(\tau)$. Then one can easily check that the state vectors $|\psi'(\tau)\rangle$ in the "adiabatic moving frame" evolve according to $|\psi'(\tau)\rangle = V^{(1)}(\tau)|\psi'(0)\rangle = V^{(1)}(\tau)|\psi_0\rangle$. Thus, in view of Eq. (8), we can express $V^{(1)}(\tau)$ directly in terms of the corresponding transformed Hamiltonian which we shall denote by $H^{(1)}(\tau)$, namely:

$$V^{(1)}(\tau) = \mathcal{T}\, e^{-\frac{i}{\hbar}\int_0^\tau H^{(1)}(t)\, dt}\ . \tag{9}$$

Since $V^{(1)}(\tau)$ is also a time-evolution operator, the same procedure may be repeated for $V^{(1)}(\tau)$. In other words, we can use $H^{(1)}(\tau)$ in place of the original Hamiltonian $H(\tau)$ to define the adiabatic part $U^{(1)}(\tau)$ of the time-evolution operator $V^{(1)}(\tau)$ and therefore write $V^{(1)}(\tau) = U^{(1)}(\tau)V^{(2)}(\tau)$. Clearly this can be continued indefinitely. The result is an *adiabatic product expansion* of the time-evolution operator:

$$U(\tau) = \prod_{i=0}^{\infty} U^{(i)}(\tau) \; . \tag{10}$$

This expression may be viewed as a generalization of the quantum adiabatic approximation [2]. This generalized quantum adiabatic approximation is carried out by calculating the first N terms in the product in (10) and approximating $U(\tau)$ by

$$\prod_{i=0}^{N} U^{(i)}(\tau) \; . \tag{11}$$

Incidentally the transformed Hamiltonian $H^{(1)}(\tau)$ may be easily obtained in the eigenbasis of the initial Hamiltonian. This is done by substituting $U^{(0)\dagger}(\tau)$ for $\mathcal{U}(\tau)$ in (8). The result is

$$\begin{aligned} H^{(1)}(\tau) &= -i\hbar \sum_{m\neq n} e^{-i[\alpha_m(\tau)-\alpha_n(\tau)]} \, A_{mn}(\tau) \, |m;0\rangle\langle n;0| \; , \\ &= i\hbar \sum_{m\neq n} e^{-i[\alpha_m(\tau)-\alpha_n(\tau)]} \, \frac{\langle m;\tau|\dot{H}(\tau)|n;\tau\rangle}{E_m(\tau)-E_n(\tau)} \, |m;0\rangle\langle n;0| \; , \end{aligned} \tag{12}$$

where $A_{mn}(\tau) := \langle m;\tau|\frac{d}{d\tau}|n;\tau\rangle$, and the second equality is obtained by differentiating Eq. (7) with respect to time and using orthonormality of the energy eigenvectors. The appearance of the time-derivative of the Hamiltonian in the expression for $H^{(1)}(\tau)$ and the fact that $H^{(1)}(\tau)$ is off-diagonal in the eigenbasis of $H(0)$ are reminiscent of the meaning of the adiabatic approximation in which $H^{(1)}(\tau)$ is neglected.

Eq. (12) can also be used to yield the transformed Hamiltonian $H^{(i+1)}(\tau)$ corresponding to the $(i+1)$-th term in (10). This is done by introducing the symbol $n^{(i)}$ which labels the eigenvectors and eigenvalues of $H^{(i)}(\tau)$, and replacing $H^{(1)}(\tau)$, n, m, $H(\tau)$ in (12) by $H^{(i+1)}(\tau)$, $n^{(i)}$, $m^{(i)}$, and $H^{(i)}(\tau)$, respectively. Clearly, $H^{(i)}(\tau)$ and consequently

$$U^{(i)}(\tau) := \sum_{n^{(i)}} e^{i\alpha_{n^{(i)}}(\tau)} \, |n^{(i)};\tau\rangle\langle n^{(i)};0| \; , \tag{13}$$

involve i-th time derivatives of the original Hamiltonian.

The generalized quantum adiabatic approximation (11) of order N is a reliable approximation for the time-evolution operator, if one can neglect $H^{(N+1)}(\tau)$. It is exact, if $H^{(N+1)}(\tau) = 0$. In fact, the latter equation may be used as a defining condition for generating a class of exactly solvable examples for which $U(\tau) = U^{(0)}(\tau)\cdots U^{(N)}(\tau)$ is the exact time-evolution operator.

In the remainder of this article, I shall demonstrate the application of the adiabatic product expansion in the analysis of the dynamics of a magnetic dipole in a changing magnetic field.

The Hamiltonian of this system is given by

$$H[R] = H(r,\theta,\varphi) = b\vec{R}(r,\theta,\varphi)\cdot\vec{J} = br(\sin\theta\cos\varphi J^1 + \sin\theta\sin\varphi J^2 + \cos\theta J^3)\ , \qquad (14)$$

where b is the Larmor frequency, (r,θ,φ) are spherical coordinates and $\vec{J}$ is the angular momentum operator with components J^μ, $\mu = 1,2,3$. The condition $r \neq 0$ guarantees the lack of level crossing. Therefore the appropriate parameter space M of this system is $\mathbb{R}^3 - \{0\}$. The time-dependence of the Hamiltonian corresponds to the curve $C : [0,T] \to M$ traced by the tip of the magnetic field in time. This curve is parametrically given by $(r(t),\theta(t),\varphi(t))$. Assuming that for all $t \in [0,T]$, $C(t) \neq (r,\theta = \pi,\varphi)$, one can choose a complete orthonormal set of single-valued eigenvectors $|n;R\rangle$ of $H[R]$. These are given by [3]:

$$|n;(r,\theta,\varphi)\rangle = |n;(r_0,\theta,\varphi)\rangle = W(\theta,\varphi)|n;(r_0,0,0)\rangle\ , \qquad \theta\in[0,\pi),\ \varphi\in[0,2\pi)\ , \qquad (15)$$

where

$$W(\theta,\varphi) := e^{-\frac{i\varphi}{\hbar}J^3}e^{-\frac{i\theta}{\hbar}J^2}e^{\frac{i\varphi}{\hbar}J^3}\ , \quad (r_0,\theta_0,\varphi_0) := (r(0),\theta(0),\varphi(0)). \qquad (16)$$

The corresponding eigenvalues are:

$$E_n(r,\theta,\varphi) = E_n(r,0,0) = \hbar\, nbr\ , \quad \text{with}\ \ n = 0,\ \pm\frac{1}{2}\ ,\ \pm 1\ ,\ \pm\frac{3}{2}\ ,\cdots\ . \qquad (17)$$

Note that in (15), $|n;(r,0,0)\rangle$ are the eigenvectors of $H(r,\theta=0,\varphi=0) = brJ^3$, i.e.,

$$J^3|n;(r,0,0)\rangle = \hbar n|n;(r,0,0)\rangle\ .$$

Assuming that the eigenvectors $|n;(r,\theta,\varphi)\rangle$ of the Hamiltonian are also eigenvectors of $|\vec{J}|^2$, i.e., they have definite angular momentum:

$$|\vec{J}|^2\,|n;(r,\theta,\varphi)\rangle = j(j+1)\,|n;(r,\theta,\varphi)\rangle\ , \qquad n = -j,-j+1,\cdots,j\ , \qquad (18)$$

one can calculate

$$
\begin{aligned}
A_{mn}(t) &= A_r^{(mn)}\,\dot r(t) + A_\theta^{(mn)}\,\dot\theta(t) + A_\varphi^{(mn)}\,\dot\varphi(t) && (19)\\
A_r^{(mn)} &:= \langle m;(r,\theta,\varphi)|\frac{\partial}{\partial r}|n;(r,\theta,\varphi)\rangle \;=\; 0\;, && (20)\\
A_\theta^{(mn)} &:= \langle m;(r,\theta,\varphi)|\frac{\partial}{\partial \theta}|n;(r,\theta,\varphi)\rangle \;=\; \frac{1}{2}\left(e^{i\varphi}C_m\delta_{m\,n-1} - e^{-i\varphi}C_n\delta_{m-1\,n}\right)\;, && (21)\\
A_\varphi^{(mn)} &:= \langle m;(r,\theta,\varphi)|\frac{\partial}{\partial \varphi}|n;(r,\theta,\varphi)\rangle\;,\\
&= i\left[m(1-\cos\theta)\delta_{mn} + \frac{1}{2}\,\sin\theta\,\left(e^{i\varphi}C_m\delta_{m\,n-1} + e^{-i\varphi}C_n\delta_{m-1\,n}\right)\right]\;, && (22)\\
H^{(1)}(t) &= \frac{1}{2}\,W(\theta_0,\varphi_0)\left[\Omega(t)\,J^+ + \Omega^*(t)\,J^-\right]W^\dagger(\theta_0,\varphi_0)\;, && (23)\\
\delta_n(t) &= -nb\int_0^t r(t')\,dt'\;, \qquad \gamma_n(t) \;=\; -n\gamma(t)\;, && (24)
\end{aligned}
$$

where $C_m := \sqrt{(j-m)(j-m+1)}$, W is defined in Eq. (16),

$$
\begin{aligned}
\Omega(t) &:= e^{-i[\alpha(t)+\varphi(t)]}\left[\sin\theta(t)\,\dot\varphi(t) + i\dot\theta(t)\right], \quad \alpha(t) \;:=\; \delta(t)+\gamma(t)\,, && (25)\\
\delta(t) &:= -b\int_0^t r(t')\,dt'\,, \quad \gamma(t) \;:=\; -\int_0^t[1-\cos\theta(t')]\,\dot\varphi(t')\,dt'\,, && (26)
\end{aligned}
$$

and extensive use is made of the properties of J^μ and $J^\pm := J^1 \pm iJ^2$, particularly:

$$
J^\pm\,|m;(r,0,0)\rangle = \hbar\,C_{\pm m}\,|m\pm 1;(r,0,0)\rangle\;.
$$

Substituting (16) and (25) in (23), and carrying out the necessary computations, one obtains:

$$
\begin{aligned}
H^{(1)}(t) &= \omega(t)\,\Big\{[\cos^2\frac{\theta_0}{2}\cos\sigma(t) - \sin^2\frac{\theta_0}{2}\cos(2\varphi_0+\sigma(t))]\,J^1 +\\
&\qquad [-\cos^2\frac{\theta_0}{2}\sin\sigma(t) - \sin^2\frac{\theta_0}{2}\sin(2\varphi_0+\sigma(t))]\,J^2 + [-\sin\theta_0\cos\sigma(t)]\,J^3\Big\}\;, && (27)\\
&=: \; b\,r^{(1)}(t)\left[\sin\theta^{(1)}(t)\cos\varphi^{(1)}(t)\,J^1 + \sin\theta^{(1)}(t)\sin\varphi^{(1)}(t)\,J^2 + \cos\theta^{(1)}(t)\,J^3\right], && (28)
\end{aligned}
$$

where $\omega(t) := |\Omega(t)| = \sqrt{\dot\theta^2 + \sin^2\theta\,\dot\varphi^2}$ is the angular speed of the tip of the magnetic field, $\sigma(t)$ is the phase of $\Omega(t)$, i.e.,

$$
\sigma(t) := -\alpha - \varphi + \xi \qquad \mod 2\pi\,,
$$

$$\cos\xi := \frac{\sin\theta\,\dot\varphi}{\omega}\,, \qquad \sin\xi := \frac{\dot\theta}{\omega}\,,$$

and $r^{(1)}(t), \theta^{(1)}(t), \varphi^{(1)}(t)$ are defined by equating the right hand sides of (27) and (28), i.e.,

$$r^{(1)}(t) \;:=\; \frac{\omega(t)\Delta(t)}{b}\,, \quad \Delta(t) \;:=\; \sqrt{1+\sin\varphi_0\sin^2\theta_0\sin[\varphi_0+2\sigma(t)]}\,, \tag{29}$$

$$\theta^{(1)}(t) \;:=\; \cos^{-1}\left[-\frac{\sin\theta_0\cos\sigma(t)}{\Delta(t)}\right]\,, \tag{30}$$

$$\varphi^{(1)}(t) \;:=\; \tan^{-1}\left[\frac{\sin\sigma(t)+\tan^2(\frac{\theta_0}{2})\sin[2\varphi_0+\sigma(t)]}{-\cos\sigma(t)+\tan^2(\frac{\theta_0}{2})\cos[2\varphi_0+\sigma(t)]}\right]. \tag{31}$$

This notation allows one to directly read off the eigenvectors $|n^{(1)};t\rangle$ and eigenvalues $E_{n^{(1)}}(t)$ of $H^{(1)}(t)$ by replacing n by $n^{(1)}$ and (r,θ,φ) by $(r^{(1)},\theta^{(1)},\varphi^{(1)})$ in Eqs. (15) and (17). Particularly interesting is the fact that $r^{(1)}(t) > 0$, unless the angular speed of the tip of the magnetic field vanishes. $\omega(t) = 0 = r^{(1)}(t)$ define the times t for which $H^{(1)}(t) = 0$. These "degenerate" situations need further treatment. Here I suffice to remind the reader that for time periods during which $H^{(1)}(t) = 0$, the adiabatic approximation is exact.

Eqs. (29)-(31) together with (15), (13), and (5) can be used to obtain $U^{(i+1)}(\tau)$ for all $i = 0, 1, \cdots$. This is done by substituting $r^{(i)},\ \theta^{(i)},\ \varphi^{(i)}$ for $r,\ \theta,\ \varphi$ in Eqs. (29)-(31), (15), (16), (5) and using (13). The result is:

$$\begin{aligned} U^{(i+1)}(\tau) \;&=\; W\left(\theta^{(i)}(\tau),\varphi^{(i)}(\tau)\right)\sum_n e^{i\alpha_{n^{(i)}}(\tau)}|n,(r_0,0,0)\rangle\langle n,(r_0,0,0)|W\left(\theta^{(i)}(0),\varphi^{(i)}(0)\right)\,, \\ &=\; W\left(\theta^{(i)}(\tau),\varphi^{(i)}(\tau)\right)\, e^{i\frac{\alpha^{(i)}(\tau)}{\hbar}J^3}\, W\left(\theta^{(i)}(0),\varphi^{(i)}(0)\right)\,, \end{aligned} \tag{32}$$

where $\alpha^{(i)}(t) := \delta^{(i)}(t) + \gamma^{(i)}(t)$ and

$$\delta^{(i)}(t) \;:=\; -b\int_0^t r^{(i)}(t')\,dt'\,, \quad \gamma^{(i)}(t) \;:=\; -\int_0^t [1-\cos\theta^{(i)}(t')]\,\dot\varphi^{(i)}(t')\,dt'\,, \tag{33}$$

$$\alpha_{n^{(i)}}(t) \;=\; n\alpha^{(i)}(t)\,, \quad \delta_{n^{(i)}}(t) \;=\; n\delta^{(i)}(t)\,, \quad \gamma_{n^{(i)}}(t) \;=\; n\gamma^{(i)}(t)\,. \tag{34}$$

For $\varphi_0 = 0$ Eqs. (29)-(31) simplify considerably. In this case one has:

$$r^{(1)}(t) = \frac{\omega(t)}{b}\,, \quad \theta^{(1)}(t) = \cos^{-1}[-\sin\theta_0\cos\sigma(t)]\,, \quad \varphi^{(1)}(t) = -\tan^{-1}\left[\frac{\tan\sigma(t)}{\cos\theta_0}\right]\,. \tag{35}$$

Substituting these relations in Eq. (33) with $i = 1$, and performing the necessary algebra, one finds:

$$\delta^{(1)}(t) \;=\; -\int_0^t v(t')dt' =: -\ell(t)\,, \quad \gamma^{(1)}(t) \;=\; -\tan^{-1}\left[\frac{X(t)+Y(t)}{1-X(t)Y(t)}\right]\,, \tag{36}$$

$$X(t) \;:=\; -\frac{\cos\theta_0[\tan\sigma(t)-\tan\sigma(0)]}{\cos^2\theta_0+\tan\sigma(t)\tan\sigma(0)}\;,\quad Y(t)\;:=\;\tan\theta_0[\sin\sigma(t)-\sin\sigma(0)]\;,\quad (37)$$

where $\ell(t)$ is the length of the projection of the portion of the curve C which lies between $C(0)$ and $C(t)$ onto the unit sphere centered at $r=0$. The appearance of such a geometric quantity in this calculation is quite remarkable.

Let us next apply the adiabatic product expansion to identify a class of exactly solvable cases. This is done by enforcing $H^{(N+1)}(\tau)=0$ or alternatively $r^{(N+1)}(\tau)=0$. The first nontrivial case is $N=1$, i.e., $r^{(2)}(\tau)=0$. This condition may be easily fulfilled by requiring $\dot\sigma=0$ which immediately leads to:

$$r(t)=\frac{1}{b}\left[\cos\theta\,\dot\varphi-\frac{\frac{d}{dt}(\frac{\dot\theta}{\sin\theta\,\dot\varphi})}{1+(\frac{\dot\theta}{\sin\theta\,\dot\varphi})^2}\right]=\frac{\dot\varphi}{b}\left[\cos\theta-\frac{\frac{d}{d\varphi}(\frac{\theta'}{\sin\theta})}{1+(\frac{\theta'}{\sin\theta})^2}\right]\;,\qquad (38)$$

where $\theta'=d\theta/d\varphi$. Thus, for every $\theta=\theta(\varphi)$ which renders the right hand side of (38) positive for all t, $|\psi(t)\rangle=U^{(0)}(t)U^{(1)}(t)|\psi_0\rangle$ is the exact solution of the Schrödinger equation (1). Clearly, one can generate further exactly solvable examples corresponding to $N=2,3,\cdots$, in this manner.

The adiabatic product expansion suggested in this article may be viewed as an iterative procedure to integrate the Schrödinger equation. It involves only algebraic manipulations and integration of scalar functions. It also provides a generalization of the quantum adiabatic approximation which involves an integer N as its order. The approximation yields the exact result if $H^{(N+1)}(\tau)=0$. In the general case where $H^{(i)}(\tau)\neq 0$, for all i, one may improve the accuracy of the approximation indefinitely by increasing its order.

As shown for the magnetic dipole system, one may be able to obtain generic expressions for the terms in the adiabatic product expansion. These can be used to generate exactly solvable examples. In particular, if the dynamics of the system is given by a dynamical group G, i.e., if the Hilbert space provides a unitary irreducible representation ρ of a Lie group G and $H(t)=\rho[h(t)]^\dagger H_d(t)\rho[h(t)]$, with $h(t)\in G$ and $H_d(t)$ diagonal, belongs to the representation of the Lie algebra of G and $U(t)=\rho[g(t)]$ for some $g(t)\in G$ [4], then one might try to employ a similar approach as the one used in the analysis of the dipole system ($G=SU(2)$). In particular this approach may be readily applied for the generalized harmonic oscillator system where $G=SU(1,1)$, [5]. An interesting direction for further study of the adiabatic product expansion is to seek its meaning and implications in the path integral approach to quantum mechanics and ultimately quantum field theory.

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